

PUBCHEM_54609806

3698-87-1 | DTXSID60715027

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.05e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.13e-01

Confidence level: 5.71e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Gluconolactone</div> <div>Measured: 3.31</div> <div>Predicted: 2.36</div>	<div>Image not found</div> <div>n,n-bis(2-cyanoethyl)aspartic acid</div> <div>Measured: 2.93e-02</div> <div>Predicted: 4.12e-02</div>	<div>Image not found</div> <div>D-Xylose</div> <div>Measured: 3.70</div> <div>Predicted: 3.35</div>
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